Real-time extension to bead-fourier path integrals

Nathan London

Contents

$$Z = \mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{H}}\right] \tag{1}$$

$$Z = \int \mathrm{d}x \left\langle x \left| \mathrm{e}^{-\beta\hat{H}} \right| x \right\rangle \tag{2}$$

$$Z \propto \int \mathrm{d}\{x_j\} \int \mathrm{d}\{p_j\}\ \mathrm{e}^{-\beta\left[\sum_{j=1}^{n}\left(\frac{nm}{2\beta^2\hbar^2}(x_{j+1}-x_j)^2+\frac{1}{n}V(x_j)\right)\right]} \tag{3}$$

$$Z = \oint D(x(u))\mathrm{e}^{-S(x(u))} \tag{4}$$

$$S(x(u)) = \frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}u \frac{m\dot{x}(u)^2}{2} + V(x(u)) \tag{5}$$

$$Z = \int \mathrm{d}x \int_{x(0)=x}^{x(\beta\hbar)=x} D(x(u))\mathrm{e}^{-S(x(u))} \tag{6}$$

$$x(u) = x + (x'-x)\frac{u}{\beta\hbar} + \sum_{k=1}^{\infty} a_k \sin\left(\frac{k\pi u}{\beta\hbar}\right) \tag{7}$$

$u_j = (j-1)\frac{\beta\hbar}{n}$ $x(u_j) = x_j$ with $x(u_{n+1}) = x_1$

$$Z = \int \mathrm{d}\{x_j\} \int_{x_1}^{x_2} D(x(u)) \cdots \int_{x_n}^{x_1} D(x(u))\mathrm{e}^{-\sum_{j=1}^{n} S_j(x(u))} \tag{8}$$

$$S_j(x(u)) = \frac{1}{\hbar}\int_{u_j}^{u_{j+1}} \mathrm{d}u \frac{m\dot{x}(u)^2}{2} + V(x(u)) \tag{9}$$

$$x_j(u) = x_j + \frac{(x_{j+1}-x_j)(u-u_j)}{u_{j+1}-u_j} + \sum_{k=1}^{\infty} a_{jk} \sin\left(\frac{k\pi(u-u_j}{u_{j+1}-u-j}\right) \tag{10}$$

$$\dot{x}(u) = \frac{dx(u)}{du} = \frac{x_{j+1}-x_j}{u_{j+1}-u_j} + \sum_k a_{jk}\frac{k\pi}{u_{j+1}-u_j}\cos\left(\frac{k\pi(u-u_j)}{u_{j+1}-u_j}\right) \tag{11}$$

$\xi = \frac{u-u_j}{u_{j+1}-u_j}$, $u_{j+1}-u_j = \frac{\beta\hbar}{n}$

$$\dot{x}(u)^2 = \left(\frac{(x_{j+1}-x_j)n}{\beta\hbar}\right)^2 + 2\frac{(x_{j+1}-x_j)n}{\beta\hbar}\sum_k a_{jk}\frac{k\pi n}{\beta\hbar}\cos(k\pi\xi) + \left(\sum_k a_{jk}\frac{k\pi n}{\beta\hbar}\cos(k\pi\xi)\right)^2 \tag{12}$$

$\int_0^1 \mathrm{d}\xi \cos(k\pi\xi) = 0$

$$\begin{aligned}\frac{1}{\hbar}\int_{u_j}^{u_{j+1}} \mathrm{d}u \frac{m\dot{x}(u)^2}{2} &= \frac{m\beta\hbar}{2\hbar n}\int_0^1 \mathrm{d}\xi\ \dot{x}(\xi)^2 \\ &= \frac{mn}{2\beta\hbar^2}\left[(x_{j+1}-x_j)^2 + \sum_k \frac{(k\pi)^2}{2}a_{jk}^2\right]\end{aligned} \tag{13}$$

$$\frac{1}{\hbar}\int_{u_j}^{u_{j+1}} \mathrm{d}u\ V(x(u)) = \frac{\beta}{n}\int_0^1 \mathrm{d}\xi\ V(x_j(\xi)) \tag{14}$$

$$Z = C(\beta)\int \mathrm{d}\{x_j\}\int \mathrm{d}\{a_{jk}\}\ \mathrm{e}^{-\beta H(x_j,a_{jk})} \tag{15}$$

$$H(x_j, a_{jk}) = \sum_{j=1}^{n}\left[\frac{mn}{2\beta^2\hbar^2}\left((x_{j+1}-x_j)^2 + \sum_{k=1}^{k_{\max}}\frac{(k\pi)^2}{2}a_{jk}^2\right) + \frac{1}{n}\int_0^1 \mathrm{d}\xi\ V(x_j(\xi))\right] \tag{16}$$

$$C(\beta) = \left(\frac{mn}{2\beta\hbar^2}\right)^{\frac{n}{2}(1+k_{\max})}\frac{k_{\max}!}{\sqrt{2}} \tag{17}$$

$$H \to H + \sum_{j=1}^{n}\left[\frac{p_j^2}{2m} + \sum_{k=1}^{k_{\max}}\frac{p_{jk}^2}{2m_k}\right] \tag{18}$$

The equations of motion for the bead-fourier system can be found as,

$$\frac{\partial p_j}{\partial t} = -\frac{\partial H}{\partial x_j}, \tag{19}$$

$$\frac{\partial x_j}{\partial t} = \frac{\partial H}{\partial p_j} = \frac{p_j}{m}, \tag{20}$$

$$\frac{\partial p_{jk}}{\partial t} = -\frac{\partial H}{\partial a_{jk}}, \tag{21}$$

and

$$\frac{\partial a_{jk}}{\partial t} = \frac{\partial H}{\partial p_{jk}} = \frac{p_{jk}}{m_k}, \tag{22}$$

with the derivative of the Hamiltonian with respect to the bead positions being

$$\frac{\partial H}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\sum_{j=1}^{n}\frac{1}{2}\omega_n^2(x_{j+1}-x_j)^2\right] + \frac{\partial}{\partial x_j}\left[\sum_{j=1}^{n}\frac{1}{n}\int_0^1 \mathrm{d}\xi\ V[x_j(\xi)]\right] \tag{23}$$

$$= \omega_n^2(2x_j - x_{j+1} - x_{j-1}) + \frac{1}{n}\left[\int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_j(\xi)]}{\partial x_j(\xi)}\frac{\partial x_j(\xi)}{\partial x_j} + \int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_{j-1}(\xi)]}{\partial x_{j-1}(\xi)}\frac{\partial x_{j-1}(\xi)}{\partial x_j}\right] \tag{24}$$

$$= \omega_n^2(2x_j - x_{j+1} - x_{j-1}) + \frac{1}{n}\left[\int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_j(\xi)]}{\partial x_j(\xi)}(1-\xi) + \int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_{j-1}(\xi)]}{\partial x_{j-1}(\xi)}\xi\right]. \tag{25}$$

The derivative of the Hamiltonian with respect to the Fourier amplitudes is

$$\frac{\partial H}{\partial a_{jk}} = \frac{1}{2}\omega_n^2(k\pi)^2 a_{jk} + \frac{1}{n}\int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_j(\xi)]}{\partial x_j(\xi)}\frac{\partial x_j(\xi)}{\partial a_{jk}} \tag{26}$$

$$= \frac{1}{2}\omega_n^2(k\pi)^2 a_{jk} + \frac{1}{n}\int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_j(\xi)]}{\partial x_j(\xi)}\sin(k\pi\xi). \tag{27}$$

$$\sum_{j=1}^{n}\frac{\partial H}{\partial x_j} = \frac{1}{n}\sum_{j=1}^{n}\int_0^1 \mathrm{d}\xi\ \frac{\partial V[x_j(\xi)]}{\partial x_j} \tag{28}$$